# Computation of pseudospectra

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**Outline:**

- **Pseudospectra**: concept
- **Computing pseudospectra**: the current approaches
- **Predictor-corrector type method**
- **Implementation**
- **Experiments**
- **Conclusions**

Trefethen: Acta Numerica, 8 (1999)

Trefethen, Embree: *Spectra and Pseudospectra* ..., 2005.

$A \in \mathbb{C}^{n \times n}$ ... **non-normal**: the classical spectral information **may be misleading**

Effects:

- transient growth for $A^k$ (discrete time stability)
- transient growth for $exp(t * A)$ (continuous time stability)
- ill-conditioned eigenvalue computations
- convergence of matrix iterations

Remedies?

**Computing pseudospectra**: early warning

$\forall \varepsilon > 0$, $\varepsilon-$**pseudospectrum** of $\mathbf{A}$

- the subset of the complex plane bounded by the $\varepsilon^{-1}$ level curve of the resolvent norm:

$$\Lambda_\varepsilon(\mathbf{A}) = \{z \in \mathcal{C} : \|(z\mathbf{I} - \mathbf{A})^{-1}\| > \varepsilon^{-1}\}$$

- the set of all complex numbers that are in the spectrum of some matrix obtained by a perturbation of norm at most $\varepsilon$:

$$\Lambda_\varepsilon(\mathbf{A}) = \{z \in \mathcal{C} : z \in \Lambda(\mathbf{A} + \mathbf{E}) \text{ for some } \mathbf{E} \text{ with } \|\mathbf{E}\| < \varepsilon\}$$

- the sets in the $z-$plane bounded by level curves of the function

$$\Lambda_\varepsilon(\mathbf{A}) = \{z \in \mathcal{C} : \ \sigma_{\text{min}}(z\mathbf{I} - \mathbf{A}) < \varepsilon\}$$

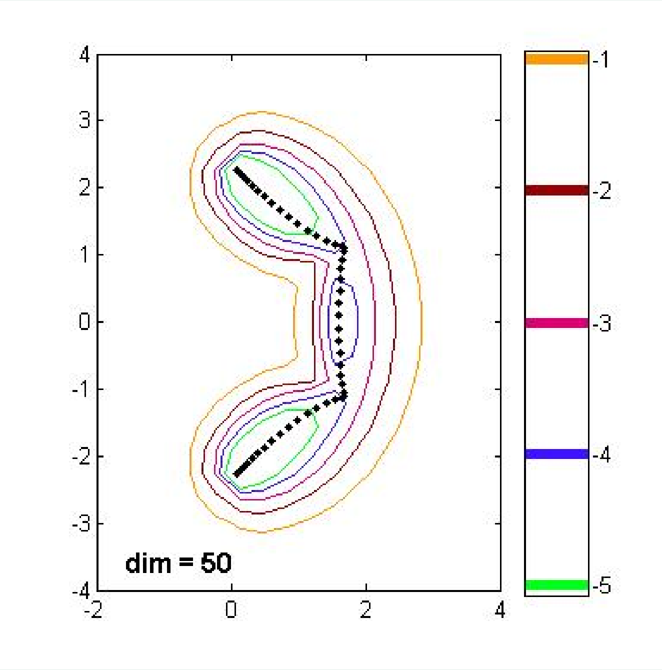
$\sigma_{\text{min}}(z\mathbf{I} - \mathbf{A})$ ... the smallest singular value of $(z\mathbf{I} - \mathbf{A})$

$\Rightarrow$ find contours

$$\partial\Lambda_\epsilon(\mathbf{A}) = \{z \in \mathcal{C} : \ \sigma_{\text{min}}\,(zI - A) = \epsilon\}$$

## **Example:** Grcar, n = 50

see http://www.comlab.ox.ac.uk/pseudospectra/eigtool




```
opts.npts = 24 ; opts.levels = [-1,-2,-3,-4,-5] ; opts.ax = [-2 4 -4 4];
[x,y] = eigtool(A,opts,figure(1))
```

## Computing pseudospectra

- Grid techniques

Trefethen: Acta Numerica, 8 (1999)
Wright: *Eigtool* ..., `http://www.comlab.ox.ac.uk/pseudospectra/eigtool`.

- Curve-tracing techniques

Brühl: BIT, 36 (1996)
Bekas, Gallopoulos: Parallel Computing, 27 (2001)
Mezher, Philippe: Numer. Alg. 29 (2002)
Burke, Lewis, Overton: IMA J. Numer. Anal., 23 (2003)
Bekas, Gallopoulos, Simoncini: submitted

Ad **grid techniques**: Select the levels i.e., the values of $\epsilon$.

1. Construct a mesh $D$ in the complex plane $\mathbb{C}$.

2. Compute $\sigma_{\text{min}}(zI - A)$ at each grid point $z \in D$.

3. Consider the level sets

$$\partial\Lambda_\epsilon = \{z \in \mathbb{C} : \sigma_{\text{min}}(zI - A) = \epsilon\}$$

for the selected values of $\epsilon$. Visualize them
as the **contour plots** on the grid.

Ad 2:
*inverse iterations* ... $(zI - A)^*(zI - A)$
*inverse Lanczos iterations* ... $(zI - A)$

Ad **curve-tracing techniques**:

**Theorem** [Sun, Brühl]: Consider $z_0 \in \partial\Lambda_\epsilon$.
Let $\sigma_{\min}$ be *simple* singular value of $z_0 I - A$. Then $\partial\Lambda_\epsilon$ is a **real analytic curve** in a neighborhood of $z_0$.
Let $u_{\min}$ and $v_{\min}$ be the relevant left and right singular vectors. Then
$\mathrm{i} v_{\min} u_{\min} / |v_{\min} u_{\min}|$
defines the anticlockwise oriented **tangent direction** at $z_0$.

**Def**: Given $z \in \mathbb{C}$, we will call
$(\sigma, u, v)$ a **singular triplet** of the matrix $zI - A$ provided that
$\sigma$ is a singular value of $zI - A$,
$u \in \mathbb{C}^n$ and $v \in \mathbb{C}^n$
are the relevant left and right singular vectors

**Def**: Given $z \in \mathbb{C}$, we will call
$(\sigma, u, v)$ a **minimum singular triplet** of the matrix $zI - A$ provided that
$\sigma$ is the smallest singular value of $zI - A$,
$u \in \mathbb{C}^n$ and $v \in \mathbb{C}^n$
are the relevant left and right singular vectors

**Algorithm** [Brühl]: Let $z_0 \in \partial\Lambda_\epsilon$. Given a fixed step size $\tau$, generate a sequence $z_k \in \mathbb{C}$ recursively as $z_{k-1} \longmapsto z_k$,

$(\sigma, u, v) =$ minimum singular triplet of $z_0 I - A$ `% initialization`

```
repeat
```

$\widehat{z}_k = z_{k-1} + \tau \mathrm{i}\,(v^* u)\,/\,|v^* u|$ `% predictor step`

$(\sigma, u, v) =$ minimum singular triplet of $\widehat{z}_k I - A$

$z_k = \widehat{z}_k - (\sigma - \epsilon)\,/\,(u^* v)$ `% corrector step`

`until` the contour is completed

**Algorithm** [Bekas, Gallopoulos] ... "Cobra", a parallel version of [Brühl]
**Algorithm** [Bekas, Gallopoulos, Simoncini] ... the projected "Cobra"
(the transfer function methodology implemented)

Shortcomings:

- the step size control ?
- the guaranteed tolerance computation ?
- the check-closed curve control ?

$\Longrightarrow$

an alternative **curve-tracing technique**:

**Problem:** Given $A \in \mathbb{C}^{n \times n}$, follow the contours

$$\partial\Lambda_\epsilon = \{z | \sigma_{\min}(zI - A) = \epsilon\}$$

**The claim:** After a "realification" and some transformations, we consider a curve

$$f : \mathbb{R}^{2+4n} \longrightarrow \mathbb{R}^{1+4n}.$$

The coordinates of the state space $\mathbb{R}^{2+4n}$ are interpreted as

- the parameter $z \in \mathbb{C}$
- $u$, $v \in \mathbb{C}^n$, respectively, are the right/left singular vectors of $(zI - A)$, related to $\sigma_{\min}(zI - A) = \epsilon$.

The pathfollowing $f$ yields the contours $\partial\Lambda_\epsilon$.

## Continuation idea

Let $B \in \mathbb{C}^{n\times n}$. Consider a *singular triplet* $(\sigma, u, v)$, $\sigma \in \mathbb{R}$, $\sigma \geq 0$, $u \in \mathbb{C}^n$, $v \in \mathbb{C}^n$ of the matrix $B$:

$$Bv = \sigma u\,, \qquad B^*u = \sigma v$$

and the *scalling conditions*

$$v^*v = 1\,, \qquad u^*u = 1\,.$$

Note that

$$\sigma u^*u = u^*Bv = (u^*Bv)^* = v^*B^*u = \sigma v^*v\,.$$

Hence, if $\sigma > 0$, the scalling is equivalent to

$$\Re(v^*v) = 1\,.$$

(or $\Re(u^*u) = 1$ or $\Re(v^*v) + \Re(u^*u) = 2$, etc.)

**Context**: $B \equiv (zI - A)$, $z = x + \mathrm{i}y$.
Let us set $\sigma = \epsilon$ ... a fixed **positive** parameter,
$u = \Re u + i\Im u$, $v = \Re v + \mathrm{i}\Im v$,

$$f : \mathbb{R}^{2+4n} \longrightarrow \mathbb{R}^{1+4n},$$

$\xi \equiv (x, y, \Re u, \Im u, \Re v, \Im v) \in \mathbb{R}^{2+4n}$,
$f(\xi) = f(x, y, \Re u, \Im u, \Re v, \Im v) \in \mathbb{R}^{1+4n} \equiv$

$$f_1(\xi) = -\epsilon \begin{bmatrix} \Re u \\ \Im u \end{bmatrix} + \begin{bmatrix} xI - \Re A & , & -yI + \Im A \\ yI - \Im A & , & xI - \Re A \end{bmatrix} \begin{bmatrix} \Re v \\ \Im v \end{bmatrix}$$

$$f_2(\xi) = -\epsilon \begin{bmatrix} \Re v \\ \Im v \end{bmatrix} + \begin{bmatrix} xI - \Re A^T, & yI - \Im A^T \\ -yI + \Im A^T, & xI - \Re A^T \end{bmatrix} \begin{bmatrix} \Re u \\ \Im u \end{bmatrix}$$

$$f_3(\xi) = (\Re v)^T \Re v + \Im v^T \Im v - 1 .$$

Generically, the equation

$$f(\xi) = f(x, y, \Re u, \Im u, \Re v, \Im v) = 0$$

defines a curve in $\mathbb{R}^{2+4n}$.

Solutions of the equation are **stratified**: Let be the curve corresponding to the $k$-th singular value (set to the fixed $\epsilon$) for $1 \leq k \leq n$ e.g.,
$k = 1$ for the largest and $k = n$ for the smallest singular value.

Let $z \in \partial\Lambda_\epsilon$ satisfy the assumption of Theorem.

$\Longrightarrow$ $f(\xi) = 0$, where $\xi = (x, y, \Re u, \Im u, \Re v, \Im v)$, $x + \mathrm{i}y = z$,
$\epsilon = \sigma_{\min}((x + \mathrm{i}y)I - A)$, $u_{\min} = \Re u + \mathrm{i}\Im u$, $v_{\min} = \Re v + \mathrm{i}\Im v$.
Hence, $\xi$ is related to a minimum singular triplet $(\epsilon, u_{\min}, v_{\min})$.

Theorem $\Longrightarrow$ $f(\xi(s)) = 0$, $s$ ... parameter (e.g. the *arclength*)

$$x(s) + \mathrm{i}y(s) = z(s),\ \epsilon = \sigma_{\min}((x(s) + \mathrm{i}y(s))I - A),$$
$$(\epsilon, u_{\min}(s), v_{\min}(s)).$$

Computational tool: **path following**

$$f : \mathbb{R}^{2+4n} \longrightarrow \mathbb{R}^{1+4n}$$

via a **predictor-corrector** technique.

Allgower, Georg: *Numerical continuation methods*, 1990.
Deuflhard: *Newton Methods for Nonlinear Problems ...* , 2004.

## Linearization: computing **oriented tangent**

Let $Df(\xi) \in \mathbb{R}^{(1+4n)\times(2+4n)}$ be differential of $f$ at $\xi$.

Let $\delta\xi \in \mathbb{R}^{2+4n}$:

$$Df(\xi)\,\delta\xi = 0\,, \qquad \delta\xi^T\,\delta\xi = 1$$

... a *tangent*

Let $(\delta x; \delta y) \in \mathbb{R}^2$ denote the first two components of $\delta\xi \in \mathbb{R}^{2+4n}$:

$$\det\begin{bmatrix} \delta x & \delta y \\ \Re(v_{\min}^* u_{\min}) & \Im(v_{\min}^* u_{\min}) \end{bmatrix} > 0\,.$$

... the *positively oriented tangent*

Here, $\xi \longleftrightarrow x + \mathrm{i}y = z$, $(\epsilon, u_{\min}, v_{\min})$.

**A starting point?**

**Problem**: Given $\epsilon > 0$, find a point $z_0 = x_0 + \mathrm{i}y_0$, $z_0 \in \partial\Lambda_\epsilon$.

Consider $(x_{\mathrm{try}}; y_{\mathrm{try}}) \in \mathbb{R}^2$, $z_{\mathrm{try}} = x_{\mathrm{try}} + \mathrm{i}y_{\mathrm{try}} \in \mathbb{C}$,
to be an **initial guess** of a point on $\partial\Lambda_\epsilon$.

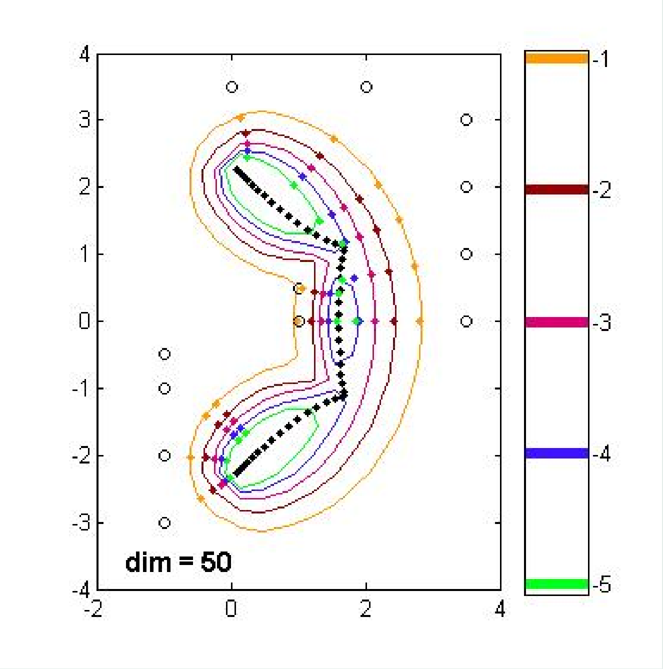
- Compute a minimum singular triplet $(\sigma_{\mathrm{min}}, u_{\mathrm{min}}, v_{\mathrm{min}})$ of the matrix $z_{\mathrm{try}}I - A$.
- Set $\xi_{\mathrm{try}} \equiv (x_{\mathrm{try}}, y_{\mathrm{try}}, \Re u_{\mathrm{min}}, \Im u_{\mathrm{min}}, \Re v_{\mathrm{min}}, \Im v_{\mathrm{min}}) \in \mathbb{R}^{2+4n}$.
Define $f$ with $\epsilon$ being set to $\epsilon \equiv \sigma_{\mathrm{min}}$. Hence, $f(\xi_{\mathrm{try}}) = 0$.
Construct positively oriented tangent $\delta\xi_{\mathrm{try}}$ at $\xi_{\mathrm{try}}$.
- Consider $f$ where $\epsilon$ is set to be the given $\epsilon > 0$. The iterations

$$\xi \to \xi - \begin{bmatrix} Df(\xi) \\ \delta\xi_{\mathrm{try}}^T \end{bmatrix} f(\xi)\,,$$

started at $\xi_{\mathrm{try}}$, are locally (quadratically) convergent to a point $\xi_0 \in \mathbb{R}^{2+4n}$, $f(\xi_0) = 0$.
- Let $(x_0; y_0) \in \mathbb{R}^2$ ... the first two components of $\xi_0$.
Let $z_0 \equiv x_0 + \mathrm{i}y_0$. Then $z_0 \in \partial\Lambda_\epsilon$.

## **Example**-continued: `Grcar`, n = 50

**testing the starting points**




**black circles** ... $z_{\text{try}} = x_{\text{try}} + \mathrm{i}y_{\text{try}} \in \mathbb{C}$
**coloured points** ... the targets of the iterations, $z_0 \in \partial\Lambda_\epsilon$
according to the scale $\epsilon = 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}$

**Computations** on `Intel T2300 1.66 GHz, dual core Centrino`,
using MATLAB version 7.1.

**Toolbox** MATCONT: A continuation software in Matlab
Dhooge, Govaerts, Kuzetsov: ACM Trans. Math. Software, 31 (2003)

Given $\epsilon > 0$: ... pointwise approximations of closed curves

$$x \equiv \{\xi_0, \xi_1, \ldots, \xi_j, \xi_{j+1}, \ldots, \xi_N\}\ , \qquad v \equiv \{\delta\xi_0, \delta\xi_1, \ldots, \delta\xi_j, \delta\xi_{j+1}, \ldots, \delta\xi_N\}\ ,$$

$\xi_j \in \mathbb{R}^{2+4n}$: $f(\xi_j) = 0$, $\delta\xi_j \in \mathbb{R}^{2+4n}$ ... positively oriented tangent, and

$$h \equiv \{\tau_0, \tau_1, \ldots, \tau_j, \tau_{j+1}, \ldots, \tau_N\}$$

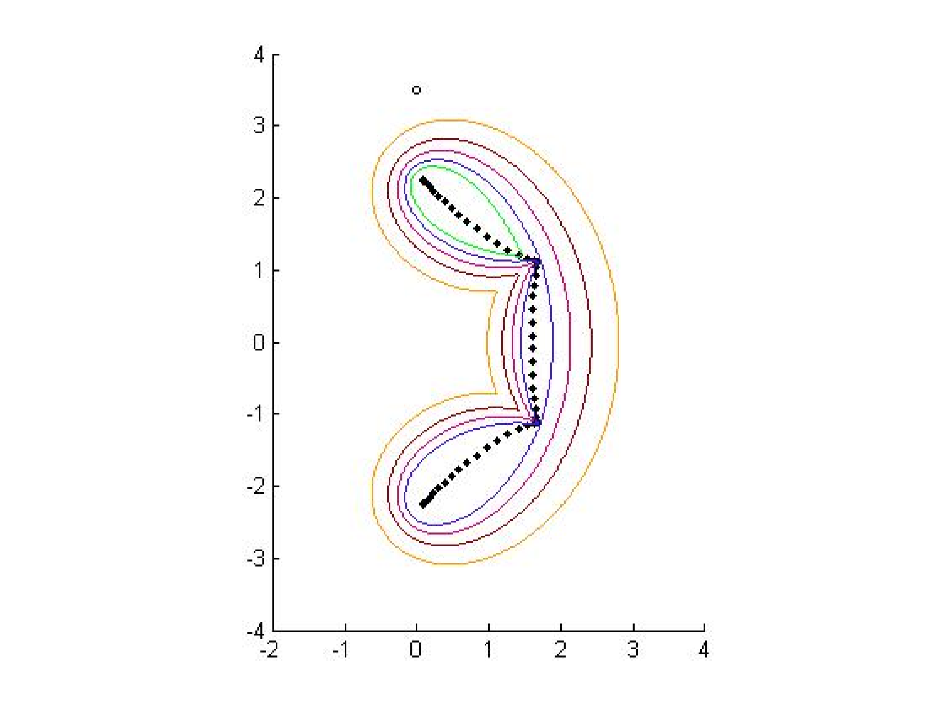
... the step-size $\tau_j$ at the $j$-th step

*predictor-corrector* algorithm: the recurrence

$$\xi_j, \delta\xi_j, \tau_j \longmapsto \xi_{j+1}, \delta\xi_{j+1}, \tau_{j+1}\ .$$

# **Example**-continued: `Grcar`, n = 50

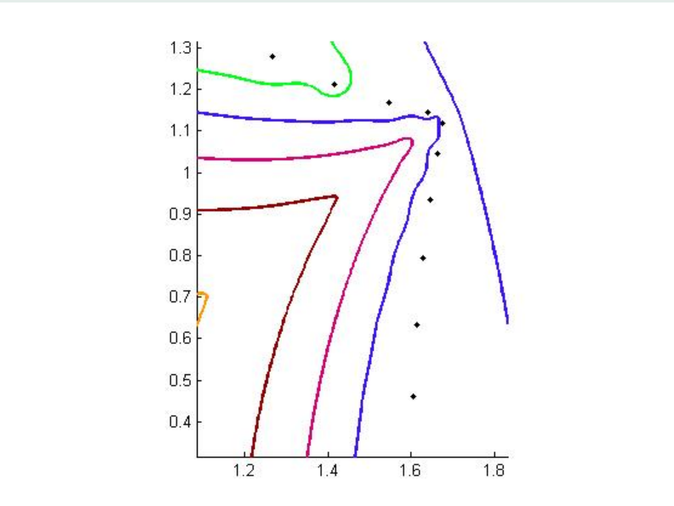
## Pathfollowing the level curves

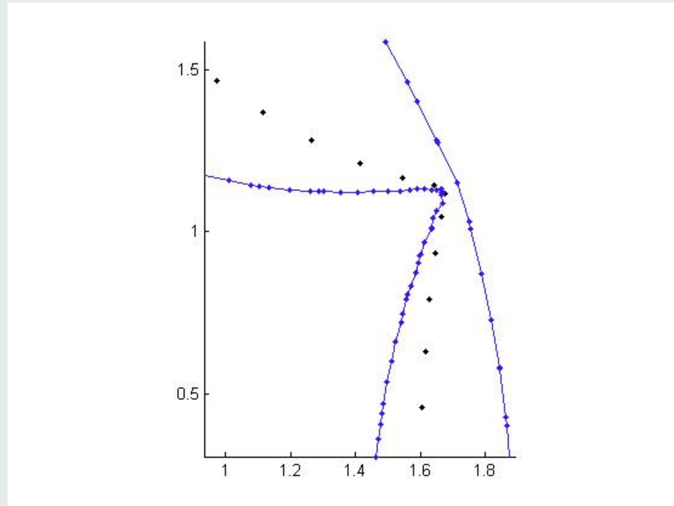



blue ... $\epsilon = 10^{-4}$

```
Closed curve detected at step 227
elapsed time = 17.3 secs, npoints curve = 227
```

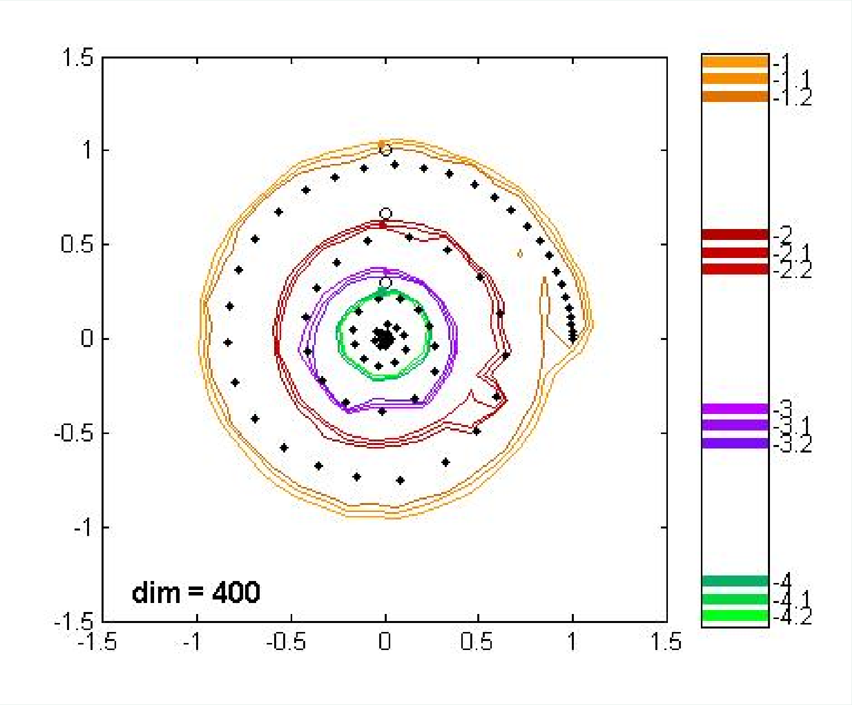
**Pathfollowing the level curves** - zoom




blue ... $\epsilon = 10^{-4}$

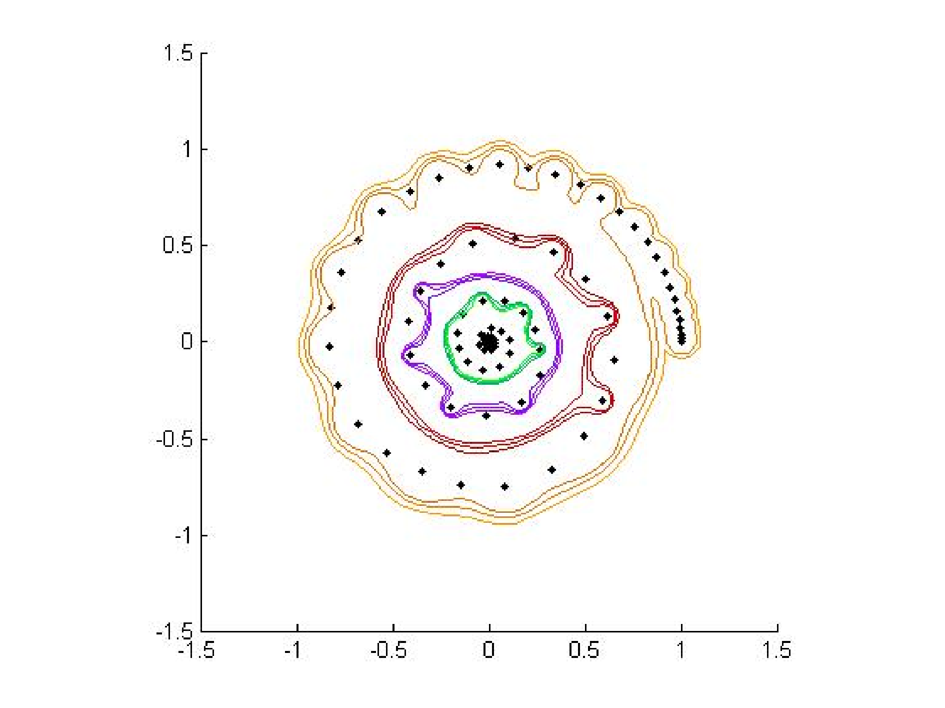
# **Example:** Landau, n = 400



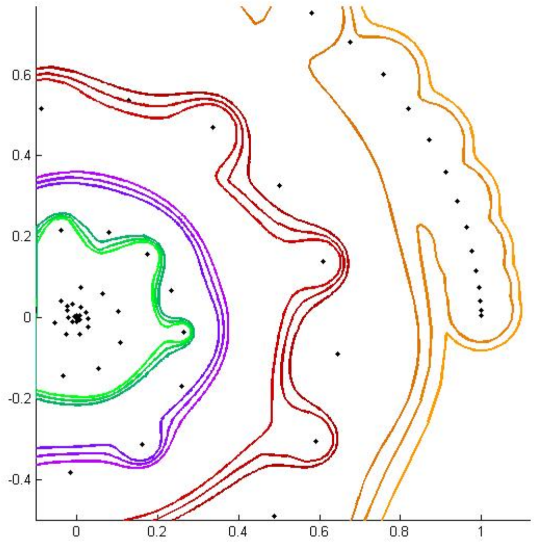

```
opts.npts = 24 ;
opts.levels = [-1,-1.1,-1.2,-2,-2.1,-2.2,-3,-3.1,-3.2,-4,-4.1,-4.2];
[x,y] = eigtool(A,opts,figure(1))
```

# Example: Landau, $n = 400$

## Pathfollowing the level curves



**Pathfollowing the level curves** - zoom



## Conclusions

- Given a matrix $A \in \mathbb{C}^{n\times n}$, we compute the branch consisting of a fixed singular value $\epsilon$ and corresponding left and right singular vectors of parameter dependent matrix $(x + \mathrm{i}y)I - A$.
- The fact that the branch corresponds to the smallest singular value $\sigma_{\min}((x + \mathrm{i}y)I - A) = \epsilon$ is sufficient to verify at just one point of the branch due to continuity argument.

- Formulation: Implicitly defined curve

$$f : \mathbb{R}^{2+4n} \longrightarrow \mathbb{R}^{1+4n}.$$

- Computational technique: the classical **predictor-corrector**.
  We can exploit standard ready-made software, just suply particular definitions of $f(\xi)$ and $Df(\xi)$.
  Hence, we may take advantage of the standard
  - step size control
  - guaranteed tolerance computation
  - check-closed curve control

**Supplemets**

- **Gallery**
- **Twists** of $u$'s and $v$'s
- **Singularites ?**

- Ad **Gallery**

## Gallery

[1] Trefethen, Embree: *Spectra and Pseudospectra ...*, 2005.
[2] Wright: *Eigtool ...*, `http://www.comlab.ox.ac.uk/pseudospectra/eigtool`.

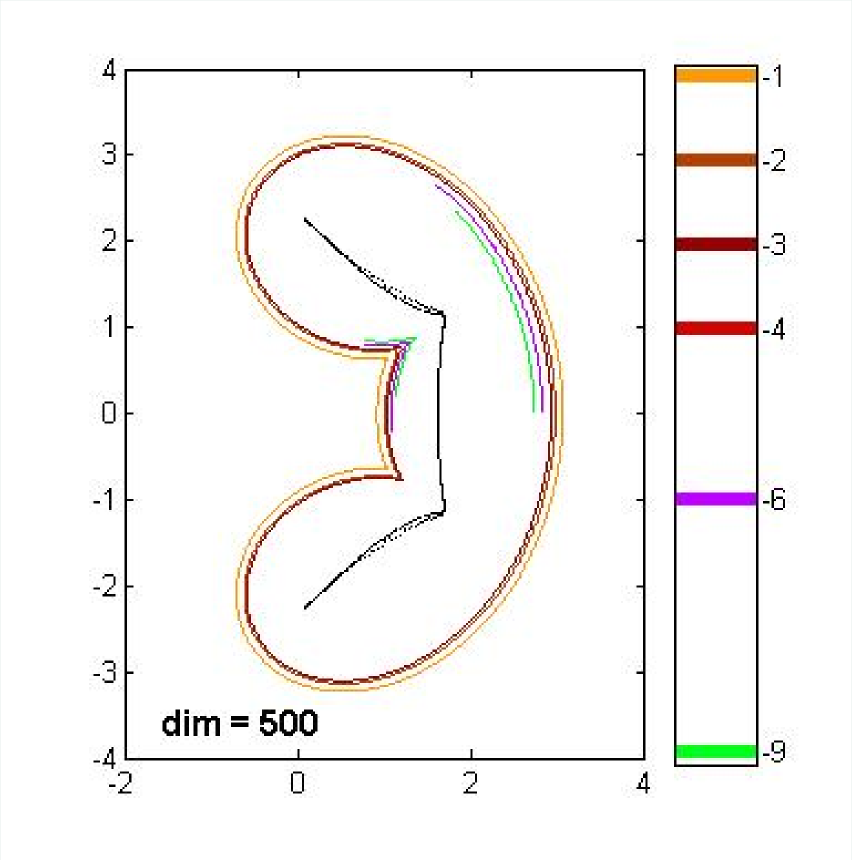
`Landau`, n = 400, $A \in \mathbb{C}^{400\times 400}$ is a full matrix
see `Landau Demo` in [2].
Motivation: see [1] § 60 (Landau: high-power lasers, unstable resonators)

`Grcar`, n = 500, $A \in \mathbb{R}^{500\times 400}$ is a sparse Toeplitz matrix
see [1] § 7, p. 58.

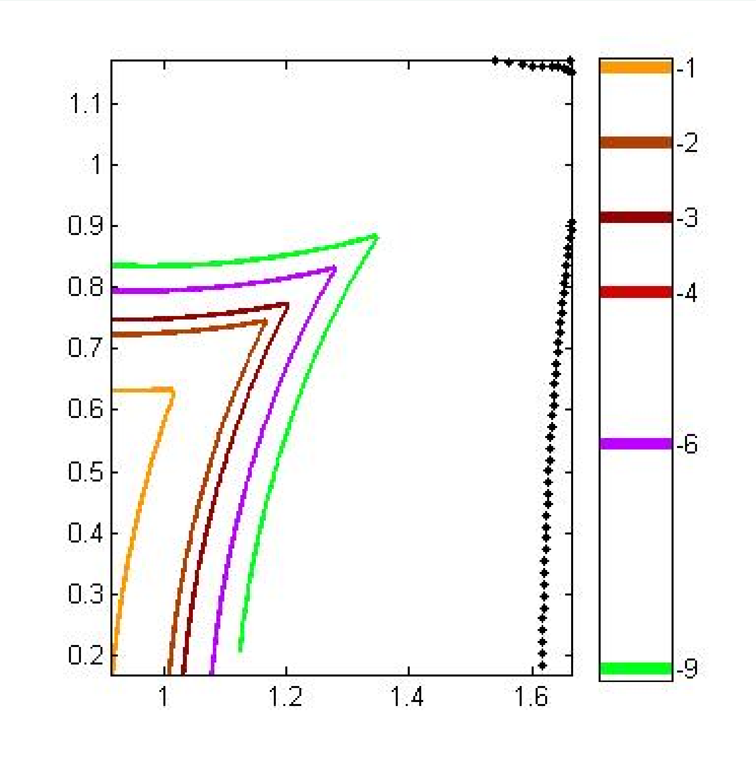
`Orr-Sommerfeld matrix`, n = 99, $A \in \mathbb{C}^{99\times 99}$ is a full matrix.
see `Orr-Sommerfeld Demo` in [2].
Motivation: see [1] § 22 (plane Poiseuille flow, Orr-Sommerfeld equation)

## Example: `Grcar`, n = 500

### Pathfollowing the level curves

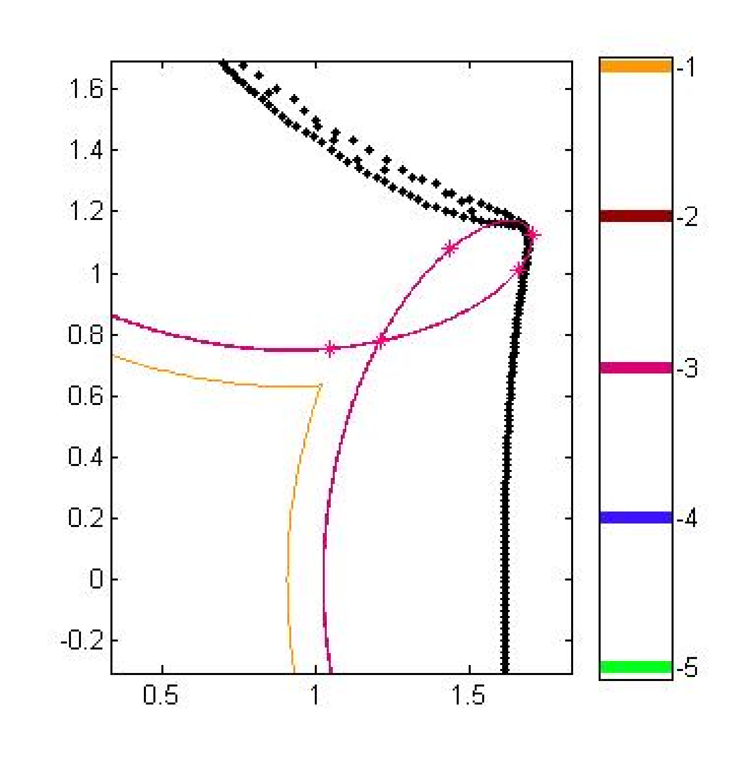


**Pathfollowing the level curves** - zoom



**Pathfollowing the level curves** - a numerical artefact

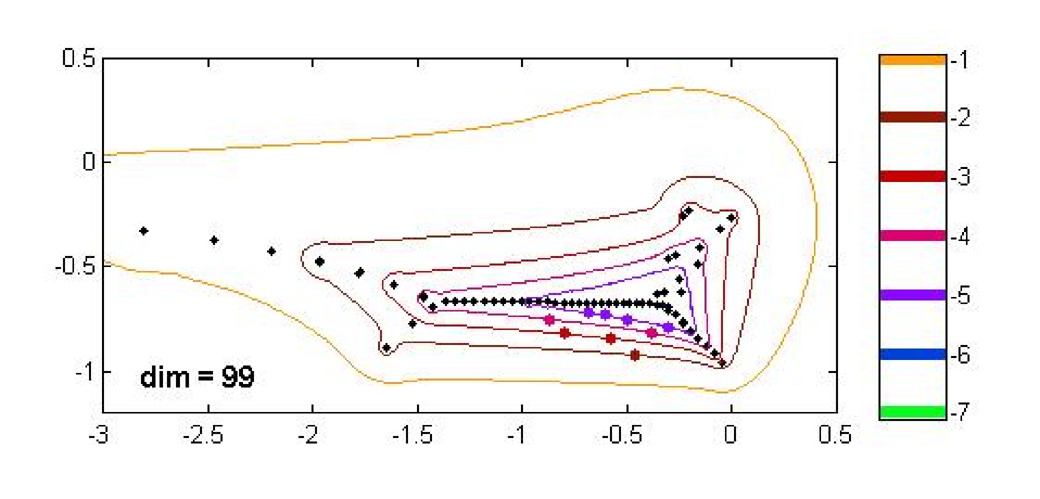
```
opt = contset(opt,'MaxStepsize', 1);
```




$\epsilon = 10^{-1}$ ... O.K., $\epsilon = 10^{-3}$ ... the quirk

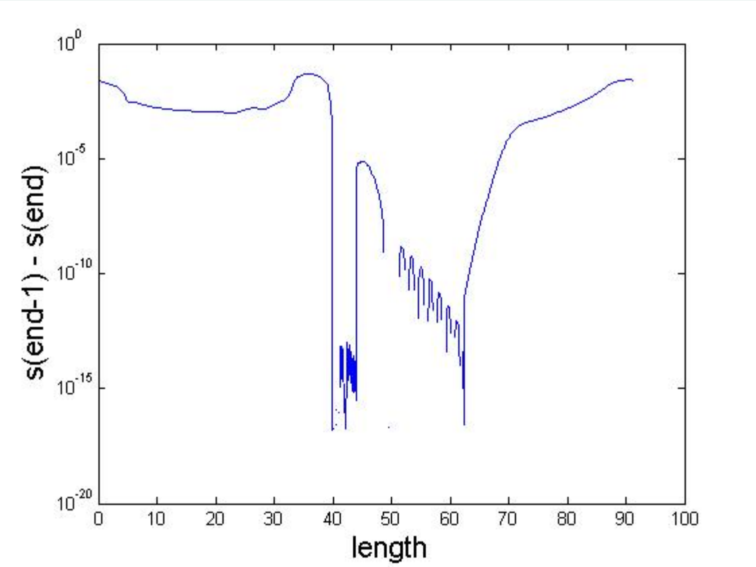
**Example:** `Orr-Sommerfeld`, $n = 99$

**Pathfollowing the level curves**



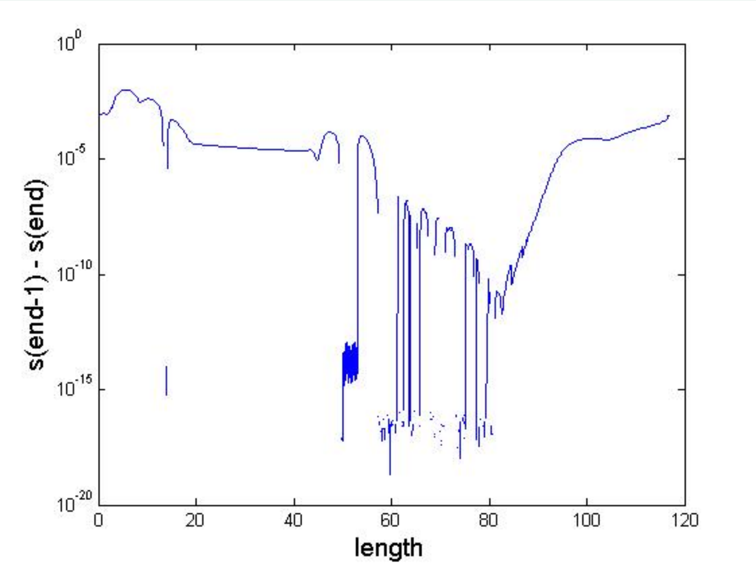

no success for $\epsilon = 10^{-6}, 10^{-7}$
restarts for $\epsilon = 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}$ marked by dots

**Restarts: explanation**




$\epsilon = 10^{-2}$
Next to the smallest $s$(end$-$1) minus
the smallest singular value $s$(end) $\equiv 10^{-2}$
vs the position on the path.

**Restarts: explanation**

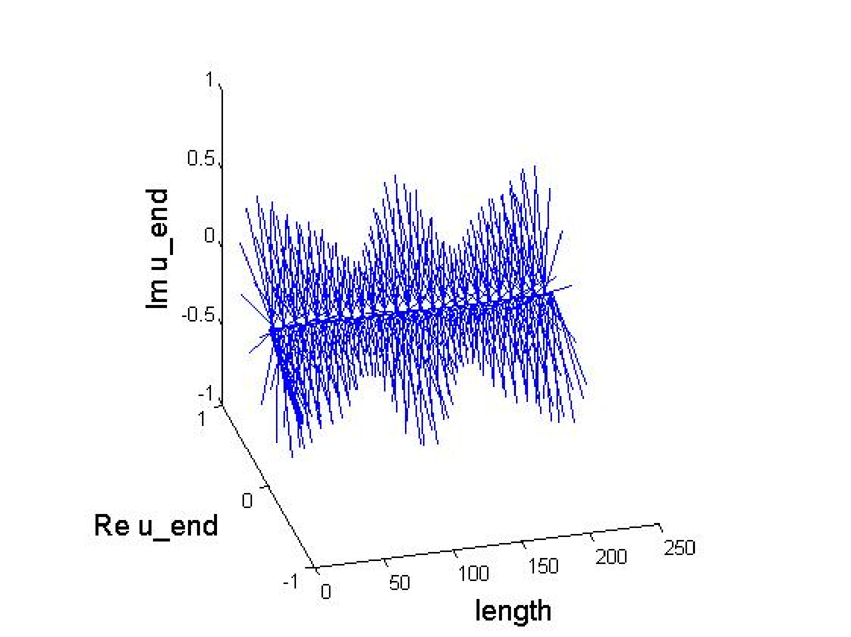



$\epsilon = 10^{-3}$
Next to the smallest $s$(end$-$1) minus
the smallest singular value $s$(end) $\equiv 10^{-2}$
vs the position on the path.

- Ad **Twists** of $u$'s and $v$'s

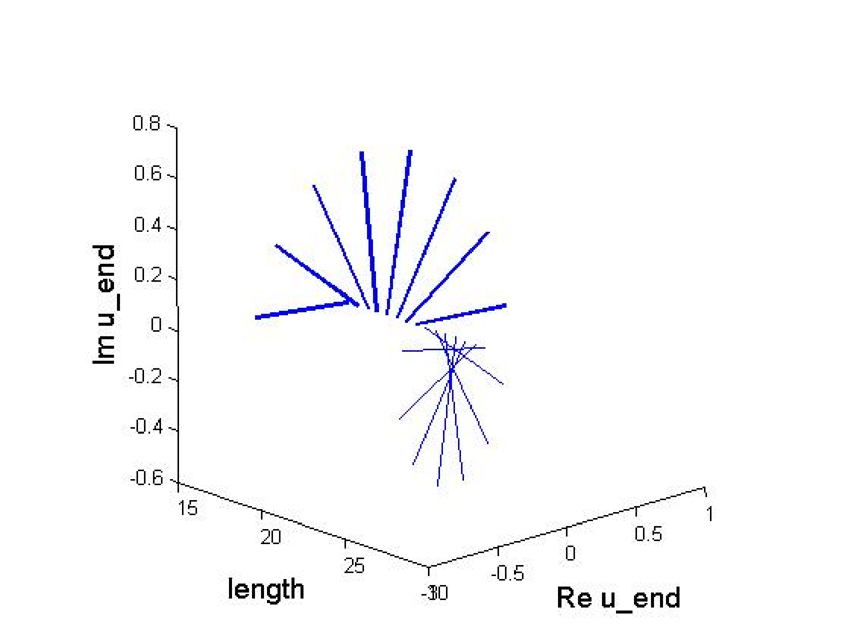
**Example:** `Grcar`, n = 50

The left singular vector $u \in \mathbb{C}^{50}$:
the last component $u_{50} = \Re u_{50} + \mathrm{i}\Im u_{50}$ vs the arclength.




$\log_{10}\epsilon = -4.1$, $z_0 = 1.4601 - \mathrm{i}\,0.0132$.

**Ad**: The last component $u_{50} = \Re u_{50} + \mathrm{i}\Im u_{50}$ vs the arclength.

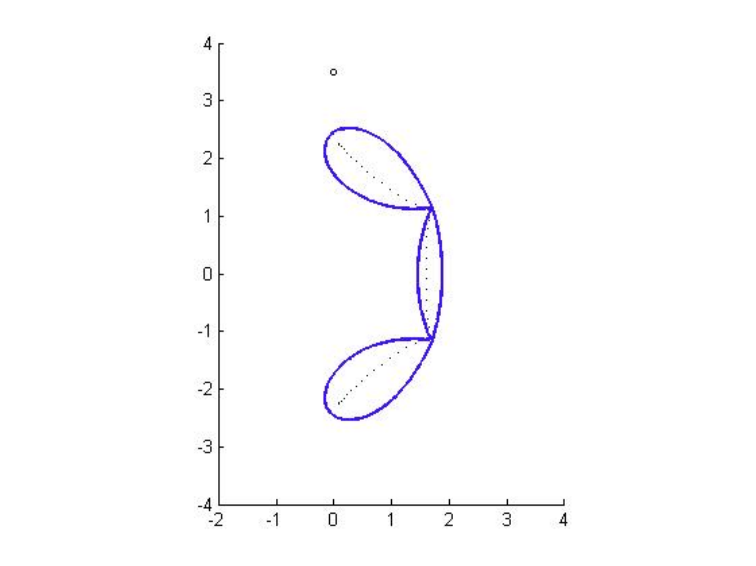


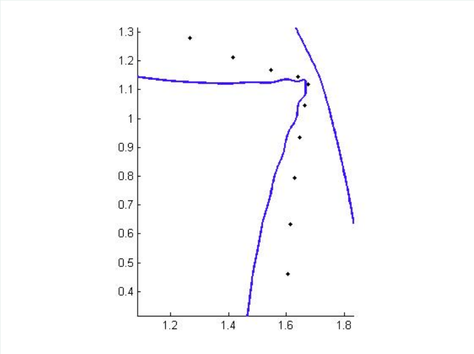

The zoom of the segment $17 \leq$ length $\leq 25$.

- Ad **Singularites ?**

Grcar, $n = 50$

**Pathfollowing the level curves**

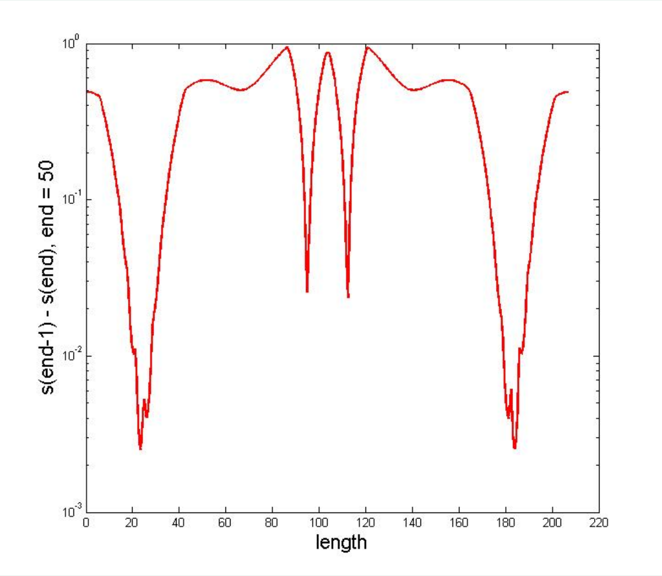



blue ... $\epsilon = 10^{-4}$

```
Closed curve detected at step 227
elapsed time = 17.3 secs, npoints curve = 227
```

Singularities?

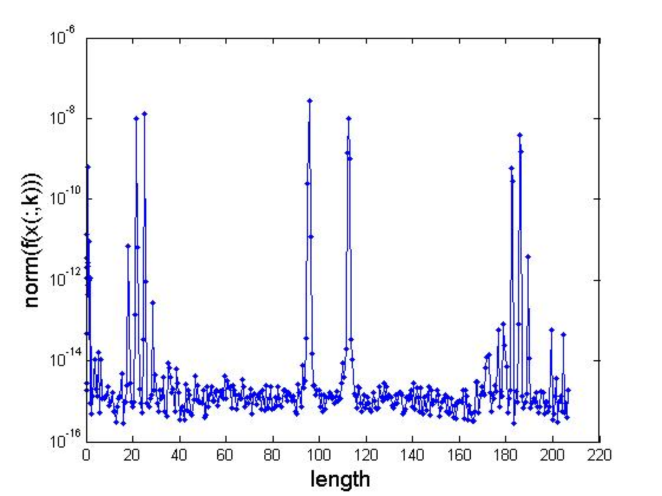



$$k \to x(:,k) \to [U,S,V] = svd(A - (x(1,k) + i * x(2,k)) * eye(n,n)) \to$$
$$\to \{s(n) \equiv \varepsilon, s(n-1)\} \to s(n-1) - s(n)$$

$k \to$ arclength

Residuum: $1 \leq k \leq 227$, $k \rightarrow$ arclength,

$$k \rightarrow \left\{z \in \mathbb{C}, u \in \mathbb{C}^{50}, v \in \mathbb{C}^{50}\right\} \equiv x \rightarrow f(x) \rightarrow \text{norm}(f(x))$$




```
opt=contset(opt,'MaxStepsize', 1);
opt=contset(opt,'MinStepsize', 1e-5);
opt=contset(opt,'InitStepsize', 0.1);
etc
```